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SOLUTION OF FINITE SYSTEMS OF EQUATIONS BY INTERVAL ITERATION.(U)

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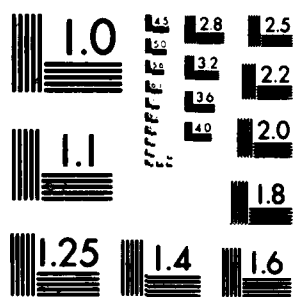
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L. B. Rall

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SOLUTION OF FINITE SYSTEMS OF EQUATIONS BY INTERVAL ITERATION

L. B. Rall

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ABSTRACT

In actual practice, iteration methods applied to the solution of finite systems of equations yield inconclusive results as to the existence or nonexistence of solutions and the accuracy of any approximate solutions obtained. On the other hand, construction of interval extensions of ordinary iteration operators permits one to carry out interval iteration computationally, with results which can give rigorous guarantees of existence or nonexistence of solutions, and error bounds for approximate solutions. Examples are given of the solution of a nonlinear system of equations and the calculation of eigenvalues and eigenvectors of a matrix by interval iteration. Several ways to obtain lower and upper bounds for eigenvalues are given.

AMS (MOS) Subject Classifications: 65G10, 65H05, 65H10, 65H15, 65F10, 65F15

Key Words: Interval analysis, Interval iteration, Linear and nonlinear systems of equations, Upper and lower bounds for solutions, eigenvalues, and eigenvectors

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## SIGNIFICANCE AND EXPLANATION

In order to complete the solution of a problem in applied mathematics and obtain the results in useful form, one must often solve a system of linear or nonlinear equations, or compute eigenvalues and eigenvectors of a matrix, which is a special case of a nonlinear system of equations. A frequently used method for solution of equations is iteration, which has been investigated extensively from a theoretical standpoint, and often applied successfully. In order to use iteration, however, one must have an initial approximation to the solution; furthermore, even if the results obtained look good, the questions of existence of a solution and accuracy of the numerical solution are not conclusively answered. By use of interval iteration, however, employing what are called computable interval extensions of ordinary iteration operators, it is possible to examine regions for existence or nonexistence of solutions, and carry out the iteration in such a way that lower and upper bounds for the solutions are given at each step and in the final result on the basis of the actual computation. Thus, questions of existence and accuracy can be answered without tedious analysis, and one can have confidence in the answers obtained by interval computation. Now that it is possible to perform interval arithmetic, for example, at speeds comparable to ordinary arithmetic, interval solution of systems of equations becomes a reliable method in problems in which accuracy is important, such as the design of structural airframes, and electrical power networks.

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## SOLUTION OF FINITE SYSTEMS OF EQUATIONS BY INTERVAL ITERATION

L. B. Rall

1. Systems of equations. Systems of  $v$  equations in  $v$  unknowns are often presented in the form

$$(1.1) \quad f(x) = 0$$

for a zero  $x = x^*$  of the operator  $f: D \subset R^v \rightarrow R^v$ , or as

$$(1.2) \quad x = \phi(x)$$

for a fixed point  $x = x^*$  of  $\phi: D \subset R^v \rightarrow R^v$ . The latter formulation will be considered here; there are many ways to transform (1.1) into an equivalent fixed point problem (1.2).

An example of a transformation of this type will be given below.

The form of (1.2) suggests the frequently-used method of *iteration*: Starting from a point  $x_0$ , in the belief that it is a more or less good approximation to  $x^*$ , the sequence  $\{x_n\}$  is generated by

$$(1.3) \quad x_{n+1} = \phi(x_n), \quad n = 0, 1, 2, \dots$$

In case (1.1) has been transformed into (1.2),  $\phi$  is often called an *iteration operator* for the solution of (1.1). In the following, it will be assumed that  $f, \phi$  and other operators considered are continuous. Under this assumption, it follows that the convergence of the sequence  $\{x_n\}$  implies the existence of a fixed point  $x^*$  of  $\phi$ , that is,

$$(1.4) \quad \lim_{n \rightarrow \infty} x_n = x^*$$

satisfies (1.2). (Of course, if  $\phi$  does not have a fixed point, then  $\{x_n\}$  cannot converge; thus, nonexistence of a fixed point  $x^*$  of  $\phi$  implies divergence of  $\{x_n\}$ .)

This is all very well, but in actual practice, one can neither represent real numbers nor perform real transformations exactly; instead of  $\{x_n\}$ , one gets a finite sequence

$\{z_n\}_{n=0}^N$  such that  $z_0 = x_0$ , but  $z_n \neq x_n$  otherwise. In order for  $\{z_n\}$  to be useful, one ordinarily has to show that  $\{x_n\}$  converges, and then produce comparisons of  $x_n$  with  $x^*$  and  $z_n$  with  $x_n$ , a problem which can be difficult in itself, or at least tedious. A more straightforward computational approach to the approximate solution of (1.2), based on the methods of interval analysis, will be given in what follows.

2. Interval analysis. Just as real analysis is concerned with the study of transformations of real numbers and vectors, interval analysis [9], [11] deals with the same for nonempty finite closed intervals

$$(2.1) \quad X = [a, b] = \{x \mid a \leq x \leq b, x \in \mathbb{R}\}$$

of real numbers, and  $n$ -tuples of such intervals, called *interval vectors*. Interval analysis is related to real analysis in two important ways. First, the real numbers can be identified with a subset of the set of real intervals (2.1), namely, the set of *degenerate* intervals with equal endpoints. For a real number  $x$ , this identification is symbolized by

$$(2.2) \quad x = [x, x].$$

Second, real transformations have *extensions* to interval transformations, as will be discussed in more detail below, and thus can be considered to be restrictions of interval transformations. In spite of this, interval analysis does not subsume real analysis, but, like complex analysis, is a distinct branch of mathematics with its own theory, techniques, and applications.

Strictly speaking, an *interval extension*  $\Phi$  of a real transformation  $\phi$  has the properties of *inclusion*

$$(2.3) \quad \Phi(X) = \{\phi(x) \mid x \in X\} \subset \Phi(X)$$

and *restriction*

$$(2.4) \quad \Phi(x) = \phi(x)$$

in the sense of (2.2). An important property of certain interval transformations is *inclusion monotonicity*:  $\Phi$  is said to be *inclusion monotone* if

$$(2.5) \quad X \subset Z \Rightarrow \Phi(X) \subset \Phi(Z).$$

Interval extensions can be formed of the operations of real arithmetic, considered as transformations from  $R^2$  into  $R$ , that is, of  $f(x,y) = x + y$ , etc., with the results forming the *interval arithmetic* of R. E. Moore [9], [11]. For example, multiplication of intervals is defined by

$$(2.6) \quad [a,b] \cdot [c,d] = [\min \Pi, \max \Pi], \quad \Pi = \{ac, ad, bc, bd\},$$

and so on. These extensions are inclusion monotone, and can be used to form inclusion monotone interval extensions of rational real functions automatically, simply by replacing the variables involved by intervals, and the arithmetic operations by their interval counterparts [9], [11].

A special class of intervals which will be useful later is the set of *symmetric* intervals, which are intervals  $S$  of the form

$$(2.7) \quad S = [-s, s] = s \cdot [-1, 1], \quad s \geq 0.$$

More generally, interval vectors and matrices are said to be *symmetric* if their components are intervals of the form (2.7). It follows from the definition of interval addition [9], [11],

$$(2.8) \quad [a,b] + [c,d] = [a+c, b+d]$$

that the sum of symmetric intervals is symmetric. Furthermore, let

$$(2.9) \quad |[a,b]| = \max\{|a|, |b|\}.$$

Then, from (2.6),

$$(2.10) \quad [a,b] \cdot [-s, s] = s |[a,b]| \cdot [-1, 1],$$

hence, multiplication of an arbitrary interval by a symmetric interval gives a symmetric interval.

Furthermore, for  $X = [a,b]$ ,  $m(X) = m([a,b]) = (a+b)/2$ ,  $w(X) = w([a,b]) = b-a$ , one can write

$$(2.11) \quad X = m(X) + \frac{1}{2}w(X) \cdot [-1, 1]$$

in terms of the *midpoint*  $m(X)$  and *width*  $w(X)$  of the interval  $X$ . The representation (2.11) of the interval  $X$  is sometimes called its *midpoint-halfwidth* or *centered form*. Multiplication of  $X$  by a real number  $\alpha$  can thus be expressed by

$$(2.12) \quad \alpha X = \alpha m(X) + \frac{1}{2}|\alpha|w(X) \cdot [-1, 1].$$



The definitions of  $|x|$ ,  $m(X)$ , and  $w(X)$  extend to interval vectors and matrices by componentwise interpretation, for example,  $m(X) = (m(X_1), \dots, m(X_v))$ , and so on. Formula (2.11) then holds without modification. Formula (2.12) extends immediately to the *inner product*  $(\alpha, X)$  of a real vector  $\alpha = (\alpha_1, \dots, \alpha_v)$  with an interval vector  $X = (X_1, \dots, X_v)$ . One has

$$(2.13) \quad (\alpha, X) = \sum_{i=1}^v \alpha_i \cdot X_i = (\alpha, m(X)) + \frac{1}{2}(|\alpha|, w(X)) \cdot [-1, 1],$$

where, of course,  $|\alpha| = (|\alpha_1|, \dots, |\alpha_v|)$ .

Interval extensions can also be made of other than rational functions, and such extensions can be combined with interval arithmetic to extend a wide class of real functions. A useful technique for obtaining interval extensions of smooth real functions is based on the *mean value form*: Suppose that  $\phi$  is (Fréchet) differentiable, and its derivative  $\phi'$  has the inclusion monotone interval extension  $\phi'$ . Then,  $\phi$  defined by

$$(2.14) \quad \phi(X) = \phi(y) + \phi'(X) \cdot (X - y), \quad y = m(X),$$

is an inclusion monotone interval extension of  $\phi$  [3], where the indicated matrix-vector operations are performed in interval arithmetic. Using (2.11), (2.14) can be written

$$(2.15) \quad \phi(X) = \phi(y) + \frac{1}{2}\phi'(X) \cdot w(X) \cdot [-1, 1], \quad y = m(X),$$

so the mean value form  $\phi(X)$  can be expressed as the sum of the real vector  $\phi(y)$  and a symmetric interval vector. This elementary observation will be useful later.

3. Interval computation. In actual practice, computing is done using a finite set  $G$  of rational numbers, rather than the set of real numbers  $R$ . Interval analysis can be adapted readily to  $G$ , which is also an ordered set. Extension of the results to be described here for one dimension can be made in a componentwise fashion to interval vectors and matrices. The key to interval computation using only elements of  $G$  is the operation of *directed rounding*, which will now be explained.

Let

$$(3.1) \quad \underline{g} = \min\{g \mid g \in G\}, \quad \bar{g} = \max\{g \mid g \in G\}.$$

Attention will be confined to the set of real numbers

$$(3.2) \quad RG = \{x \mid \underline{g} \leq x \leq \bar{g}, x \in R\},$$

and attempts to compute a real number  $z$  such that  $z < \underline{g}$  or  $z > \bar{g}$  will be said to result in an error condition called *overflow*. (Alternatively, the extended real numbers  $\pm\infty$  could be adjoined to  $G$ , with overflow detected in case the result of a computation is a semi-infinite or infinite interval.) Now,  $IG$  will denote the set of all intervals with endpoints in  $G$ , that is,

$$(3.3) \quad IG = \{[a,b] \mid a \leq b, a,b \in G\}.$$

This is the set of intervals which are *exactly representable* in terms of the numbers which are available in the actual computation. For  $x \in RG$ , the *upward rounding operator*  $\Delta$  to  $G$  is defined by

$$(3.4) \quad \Delta x = \min\{g \mid g \geq x, g \in G\},$$

and the *downward rounding operator*  $\nabla$  to  $G$  by the corresponding expression,

$$(3.5) \quad \nabla x = \max\{g \mid g \leq x, g \in G\}$$

[7]. For the set  $IRG$  of intervals with endpoints in  $RG$ , application of the *directed rounding operator*  $\square$  to intervals  $[a,b] \in IRG$  gives

$$(3.6) \quad \square[a,b] = [\nabla a, \Delta b] \in IG,$$

and thus  $\square$  maps  $IRG$  into  $IG$ . Furthermore, it is clear that  $\square$  is an inclusion monotone interval transformation, and that the interval defined by (3.6) is the element of  $IG$  of minimum width which contains  $[a,b]$ . If  $x \in RG$  is a real number, then

$$(3.7) \quad \square x = [\nabla x, \Delta x]$$

will be called the *representation* of  $x$  in  $IG$  of minimal width. If  $[\nabla x, \Delta x] = [c,d]$  is nondegenerate, then  $[c,d]$  also represents each real number  $z$  such that  $c < z < d$  in this way.

Thus, if  $\phi$  is an interval transformation which maps  $IRG$  into  $IRG$ , then the corresponding *rounded transformation*

$$(3.8) \quad F = \square\phi$$

maps IRG (and hence IG) into IG. Interval transformations  $F: D \subset IG \rightarrow IG$  are said to be *computable* on G; furthermore, if F has property (2.3) (inclusion of the real transformation  $\phi$ ) and (2.5) (inclusion monotonicity), then F will be called a *computable interval extension* of  $\phi$ . It follows that one can start with an interval transformation  $\phi: D \subset IRG \rightarrow IRG$  with properties (2.3) and (2.5) (in particular,  $\phi$  can be an inclusion monotone interval extension of  $\phi$ ), and obtain the computable interval extension (3.8) of  $\phi$  by applying the rounding operator  $\square$ . This construction can be carried out automatically if interval arithmetic and a library of computable interval extensions of the real functions entering into the definition of  $\phi$  are available. One problem which arises in this connection is that many computers lack the roundings (3.4) and (3.5) required to support interval arithmetic. This defect can be remedied by software [25], [26] or microprogramming [13], if necessary. The scientific computing language PASCAL-SC [8] includes properly rounded interval arithmetic as a standard feature. Henceforth, all interval transformations considered will be assumed to be computable.

4. Interval iteration. A standard approach to the solution of equation (1.1) by interval methods is to transform it into a fixed point problem (1.2) in some way, and then apply *interval iteration* [1], [12]. This process takes the following form:

Given an interval transformation  $\phi$  which includes  $\phi$  in the sense of (2.3), and an interval  $X_0$  thought to contain a fixed point  $x^*$  of  $\phi$ , the sequence of intervals  $\{X_n\}$  defined by

$$(4.1) \quad X_{n+1} = X_n \cap \phi(X_n), \quad n = 0, 1, 2, \dots,$$

is generated. The following results are well known [24]:

(i) If  $x^* \in X_0$ , then

$$(4.2) \quad x^* \in X = \bigcap_{n=0}^{\infty} X_n,$$

so that existence of a fixed point of  $\phi$  in  $X_0$  implies convergence of (4.1) in the sense that  $X \neq \emptyset$ , the empty set.

(ii) If, for some positive integer N,

$$(4.3) \quad X_N = \emptyset,$$

then the interval  $X_0$  contains no fixed point  $x^*$  of  $\phi$ . Hence, divergence of (4.1) in the sense of (4.3) implies nonexistence of a fixed point of  $\phi$  in  $X_0$ ; this is the contrapositive of the assertion in (i).

In finite dimensions, one has further:

(iii) If

$$(4.4) \quad \phi(X_M) \subset X_M$$

for some finite integer  $M$ , then there exists a fixed point  $x^*$  of  $\phi$  in  $X_M$ , and (4.2) holds as a consequence [10]. This is because (4.4) implies that the continuous operator  $\phi$  maps the closed compact region  $X_M$  into itself, and thus  $x^* \in X_M \subset X_0$  by the Schauder fixed point theorem.

Moreover, if  $x^* \in X_0$  is a fixed point of  $\phi$ , and  $X_n = [\underline{x}_n, \bar{x}_n]$ ,  $X = [\underline{x}, \bar{x}]$ , then one has the lower and upper bounds,

$$(4.5) \quad \underline{x}_n \leq x^* \leq \bar{x}_n, \quad n = 0, 1, 2, \dots, \quad \text{and} \quad \underline{x} \leq x^* \leq \bar{x},$$

where the inequalities are interpreted componentwise in several dimensions. From (4.5), approximations to  $x^*$  and guaranteed error bounds can be obtained easily, if desired.

The above theory requires no modification in case the calculations are performed on a finite set of points  $G$  in one or more dimensions by taking a computable interval extension  $\phi$  of  $\phi$ , and the initial interval  $X_0 \in IG$ . In this case, however, the interval iteration process (4.1) is *finite*, and will *terminate* in either the condition (4.3), establishing nonexistence of  $x^*$  in  $X_0$ , or

$$(4.6) \quad X_{N+1} = X_N \neq \emptyset$$

in which case  $X = X_N$  in (4.2). Condition (4.6) is called the *Nickel termination criterion* [15]. The upper bound

$$(4.7) \quad N \leq G\#(X_0)$$

has been given for  $N$  [24], where  $G\#(X_0)$  denotes the number of points of  $G$  contained in  $X_0$ .

Interval iteration is thus an *observable* process in actual computation, since

it yields a finite sequence  $\{X_n\}_{n=0}^N$ , the usefulness of which can often be determined by inspection. One gets nonexistence of  $x^*$  if (4.3) holds, or existence if (4.4) is true for  $M \leq N$ , and the guaranteed bounds (4.5) if  $X_0$  contains one or more fixed points  $x^*$  of  $\phi$ . One is in the dark concerning existence, however, if (4.6) holds without (4.4) occurring along the way. In particular, if  $X_0 \subset \phi(X_0)$  properly, then  $X_1 = X_0 = X$ , and the interval iteration is said to have *stalled*. The difficulty concerning existence can be resolved by applying some other existence test than (4.4) to  $X = X_N$ , a region which will be smaller than  $X_0$  unless the iteration stalled, or  $X$  can be divided into subregions for further investigation, using the algorithm of Moore and Jones, which has also been shown to be finite if  $G$  is sufficiently fine [13], [14].

5. An interval iteration operator. A simple way to convert the equation (1.1) to be solved into a fixed point problem (1.2) is by introduction of the *iteration operator*  $\phi$  defined by

$$(5.1) \quad \phi(x) = x - Yf(x),$$

where  $Y$  is a nonsingular real matrix, in which case the two problems are equivalent. Supposing that  $f$  has the (Fréchet) derivative  $f'$ , represented by the *Jacobian matrix*  $f'(x) = (\partial f_i(x)/\partial x_j)$  [20], then  $\phi$  will also be differentiable, with

$$(5.2) \quad \phi' = I - Yf',$$

where  $I$  denotes the identity matrix. The derivative (5.2) can be used to construct the mean value form (2.7) of  $\phi$ , provided that  $f'$  has an inclusion monotone interval extension  $F'$ , so that  $K$  defined by

$$(5.3) \quad K(X) = y - Yf(y) + \{I - YF'(X)\} \cdot (X - y), \quad y = m(X),$$

will be an inclusion monotone interval extension of the iteration operator  $\phi$  in (5.1).  $K$  is often called the *Krawczyk operator* [5].

An alternative form of the Krawczyk operator (5.3) can be obtained by the use of (5.1) and (2.15). One has

$$(5.4) \quad K(X) = \phi(m(X)) + \{I - YF'(X)\} \cdot w(X) \cdot \frac{[-1,1]}{2},$$

which expresses  $K(X)$  as the sum of the *iteration point*  $\phi(y)$  of  $y = m(X)$  and a symmetric interval vector. Some specific choices of the real matrix  $Y$  will now be examined.

(i) An ideal choice of  $Y$  is  $Y = [f'(x^*)]^{-1}$ , the inverse of the Jacobian matrix of  $f$  at a solution  $x = x^*$  of equation (1.1). For this fixed matrix, the ordinary iteration process (1.3) with  $\phi$  given by (5.1) will converge quadratically for  $x_0$  in some neighborhood  $N(x^*)$  of  $x^*$  [19]. This gives the possibility of quadratic convergence of the endpoints of  $X_n$  to  $x^*$ , at least for  $X_0 \subset N(x^*)$ . Of course, since  $x^*$  is unknown, it is usually not possible to find  $f'(x^*)$ . However, if  $f'$  satisfies an equation of the form  $f'(x) = h(f(x))$ , then one has  $f'(x^*) = h(0)$ , and  $Y$  can be found without knowing  $x^*$ , thus giving a rapidly convergent iteration method of simple form [19]. A numerical example of this type, in which the interval iteration converges quadratically, will be given below.

(ii) By analogy with Newton's method [5], one can choose, if it exists,

$$(5.5) \quad Y = [f'(y)]^{-1} = [f'(m(X))]^{-1}.$$

In this case, the iteration point  $\phi(m(X))$  will be the same as obtained by applying one step of the Newton iteration process to (1.1), starting from  $x_0 = y = m(X)$ . The corresponding interval iteration operator  $K$  defined by

$$(5.6) \quad K(X) = \phi(m(X)) + \{I - [f'(m(X))]^{-1}F'(X)\} \cdot w(X) \cdot \frac{[-1,1]}{2}$$

will be called the *Newton form* of the Krawczyk iteration operator defined by (5.4).

It should be noted that the discussion of interval iteration in §4 also applies to the case in which  $Y$  depends on  $X$  as long as  $\phi(X)$  contains  $\phi(X)$  for an operator  $\phi$  with fixed point  $x^*$ , in particular, for  $\phi$  as given by (5.1).

(iii) Another possible choice of  $Y$  is

$$(5.7) \quad Y = [m(F'(X))]^{-1},$$

again provided that the indicated inverse exists. Writing

$$(5.8) \quad F'(X) = m(F'(X)) + \frac{1}{2}w(F'(X)) \cdot [-1,1]$$

by (2.11), substitution into (5.4) yields, with the aid of (2.12),

$$(5.9) \quad K(X) = \phi(m(X)) + [m(F'(X))]^{-1} |w(F'(X))w(X)| \cdot \frac{[-1,1]}{4},$$

where  $|Y| = (|y_{ij}|)$  for the real matrix  $Y = (y_{ij})$ . The interval operator  $K$  defined

by (5.9) will be called the *Moore-Jones form* of the Krawczyk iteration operator [14]. Compared to (5.6), (5.9) has the computational advantage that the elements of  $m(F'(X))$  can be obtained by simple arithmetic once  $F'(X)$  has been formed, while construction of  $f'(m(X))$  requires the computation of the  $v^2$  elements of the  $v \times v$  Jacobian matrix  $f'(y)$ . (A case in which the two operators coincide will be considered later.)

The Krawczyk operator is useful in two ways in connection with ordinary iteration:

(i)  $K$  may be used to test an interval  $X$  for the existence or nonexistence of a solution  $x^* \in X$  or (1.1), according as  $K(X) \subset X$  or  $K(X) \cap X = \emptyset$  [14]. In case this test shows that  $x^* \in X$ , this establishes the suitability of  $x_0 = y = m(X)$  as a starting point for the ordinary iteration (1.3) under fairly mild conditions [14]. On the other hand, given  $y = x_0$ , one may take  $X = X_\rho$  to be the cube with diameter  $2\rho$  (in the  $l_\infty$  norm for  $R^v$ ) centered on  $y$ ,

$$(5.10) \quad X_\rho = y + \rho e \cdot [-1, 1],$$

for which (5.6) and (5.9) become

$$(5.11) \quad K(X_\rho) = \phi(y) + \rho \{I - [f'(y)]^{-1} F'(X_\rho)\} e \cdot [-1, 1],$$

where  $e = (1, 1, \dots, 1)$ , and

$$(5.12) \quad K(X_\rho) = \phi(y) + \frac{\rho}{2} [m(F'(X_\rho))]^{-1} w(F'(X_\rho)) e \cdot [-1, 1],$$

respectively. These are very simple to compute, since the formation of the product  $Ae$  for a real or interval matrix  $A$  does not require any multiplications;  $Ae$  is simply the vector consisting of the sums of the rows of  $A$ .

If one wishes to examine  $K(X_\rho)$  for several values of  $\rho$ , then the Newton form (5.11) has the computational advantage that  $[f'(y)]^{-1}$  remains fixed, while  $m(F'(X_\rho))^{-1}$  must be recalculated in the Moore-Jones form (5.12) for each  $\rho$ .

(ii)  $K$  may be used to determine the accuracy of the elements of an ordinary iteration sequence  $\{x_n\}$ . In this case, for  $y = x_n$ ,  $\phi(y) = x_{n+1}$ . A choice of  $\rho$  which is supported by the Kantorovich theory for the convergence of Newton's method [21] is  $\rho = 2r_n$ , where

$$(5.13) \quad r_n = \|x_n - \phi(x_n)\|_\infty = \|x_n - x_{n+1}\|_\infty, \quad n = 0, 1, 2, \dots$$

If  $K(X_\rho) \subset X_\rho$  for this (or other) choice of  $\rho$ , then the existence of  $x^*$  is verified, and one has the error bounds

$$(5.14) \quad \|x^* - x_n\|_\infty \leq \rho, \quad \|x^* - x_{n+1}\|_\infty \leq \frac{1}{2}w(K(X_\rho)),$$

since  $x^* \in K(X_\rho) \subset X_\rho$ . From (5.12),

$$(5.15) \quad \|x^* - x_{n+1}\|_\infty \leq \frac{\rho}{2} \| [m(F'(X_\rho))]^{-1} \| w(F'(X_\rho)) \|_\infty,$$

and (5.11), (5.12), or, more generally, (5.6), also give componentwise bounds for  $x^* - x_{n+1}$ .

Thus, the interval iteration operator  $K$  can be *preapplied* to scout for a likely region in which ordinary iteration will converge to a fixed point, or *postapplied* to verify the existence of  $x^*$  and obtain error bounds for a result obtained by ordinary iteration, perhaps computed only approximately. In this respect, the Krawczyk operator (5.3) requires a slight modification for computation on a finite set  $G$ . Suppose that  $F$  is a computable interval extension of  $f$ , and  $F'$  is a computable interval extension of  $f'$ . Then, one can use  $K$  defined by

$$(5.16) \quad K(X) = y - YF(y) + \{I - YF'(X)\} \cdot (X - y),$$

where all arithmetic operations indicated are performed in correctly rounded interval arithmetic. One can write  $a \boxplus b = \square(a + b)$  for interval addition followed by directed rounding, etc. The directed rounding operator  $\square$  will be suppressed, however, for clarity of notation, and its use will be understood in connection with actual computation. The computable transformation (5.16) will include the interval transformation (5.3), which is all that is required for the purpose of interval iteration. It is also possible to construct a computable interval extension of  $K$  which is inclusion monotone on subsets of  $X_0$ . Suppose that for each  $y \in X_0$ , one can find  $z(y) \in G$  such that

$$(5.17) \quad \phi(y) \in z(y) + \epsilon \cdot [-1, 1]$$

for some fixed  $\epsilon > 0$ . Then, from (5.4),

$$(5.18) \quad K(X) = z(y) + \{I - YF'(X)\} \cdot \frac{1}{2}w(X) + \epsilon \cdot [-1, 1]$$

is a computable interval extension of the Krawczyk operator which has the property



$X \subset Z \subset X_0 \Rightarrow K(X) \subset K(Z)$ , which will be called *inclusion monotonicity on subsets of*  $X_0$ . Since interval iteration stays entirely within the initial interval  $X_0$ , this is satisfactory for practical purposes.

For the Moore-Jones transformation (5.12), this enlargement of the Krawczyk transformation takes the simple form

$$(5.19) \quad K(X_0) = z(y) + \{eI + \frac{\rho}{2}|Y|w(F'(X_0))\}e \cdot [-1,1]$$

where  $[m(F'(X_0))]^{-1} \in Y$ . Thus, once  $F'(X_0)$  and  $Y$  have been obtained, the only interval operation to be performed in the evaluation of (5.19) is the trivial multiplication by  $[-1,1]$ ; the rest can be done with properly rounded real arithmetic. In particular, calculation of the components of the vector  $\{eI + \frac{\rho}{2}|Y|w(F'(X_0))\}e$  requires only operations with non-negative numbers and upward rounding (3.4). Recall that  $|Y|$  is defined componentwise by (2.9).

6. Interval iteration with fixed  $Y$ . What will be considered here is interval iteration with the simple case (i) of the Krawczyk transformation defined in §5, in which the matrix  $Y$  remains fixed. One would like, of course, to have  $Y = [f'(x^*)]^{-1}$ , or an approximation to the inverse of the Jacobian matrix of  $f$  at  $x = x^*$ , a solution of equation (1.1). This is possible in the special case that (1.1) is a *linear* system of equations, that is,  $f$  is an *affine* operator given by

$$(6.1) \quad f(x) = Ax - c,$$

where  $A$  is a nonsingular matrix and  $c$  is a given vector. Here,

$$(6.2) \quad f'(x) = A,$$

a constant operator [20], and thus  $[f'(x^*)]^{-1} = A^{-1}$ . With this choice of  $Y$ , it follows from (5.3) that  $K(X_0) = x^*$ , and thus the interval iteration will converge to the solution  $x = x^*$  of  $Ax = c$  in one step for arbitrary  $X_0$  such that  $x^* \in X_0$ . In practice,  $Y$  will only be an approximation to  $A^{-1}$ . Because of (6.2), one can take  $F'(X) = A$  for arbitrary  $X$ , and thus (5.4) becomes

$$(6.3) \quad K(X) = m(X) - Y(Am(X) - c) + \{I - YA\}w(X) \cdot \frac{[-1,1]}{2},$$

or, in case  $X$  is taken to be a cube  $X_0 = y + \rho e \cdot [-1,1]$ , one has

$$(6.4) \quad K(X_p) = y - Y(Ay - c) + \rho[I - YA]e \cdot [-1, 1],$$

which is a very simple interval transformation to calculate. The *residue*  $r = f(y) = Ay - c$  enters into (6.4) in a natural way.

In connection with the solution of linear equations, it should be noted that intervals *do not* form a linear space. From the rule for subtraction [9], [11],

$$(6.5) \quad [a, b] - [c, d] = [a - d, b - c],$$

it follows, for example, that

$$(6.6) \quad [0, 1] - [0, 1] = [-1, 1].$$

Thus, techniques from algebra which depend on linearity cannot be expected to extend to interval analysis, since a linear substructure is not present. Some failures in attempted solution of linear systems by interval versions of methods from linear algebra are due to a lack of understanding of this fact, not to a defect of interval analysis.

For an example of a simple system of nonlinear equations to which the method of this section applies, consider the equations

$$(6.7) \quad \begin{aligned} \exp(-u + v) - 0.1 &= 0, \\ \exp(-u - v) - 0.1 &= 0, \end{aligned}$$

due to Cuyt and Van der Cruyssen [4] for  $x = (u, v) \in \mathbb{R}^2$ . (Perhaps this system is too simple; an equivalent linear system can be obtained by taking logarithms.) The Jacobian matrix corresponding to (6.7) is

$$(6.8) \quad J(u, v) = \begin{pmatrix} -\exp(-u + v) & \exp(-u + v) \\ -\exp(-u - v) & -\exp(-u - v) \end{pmatrix}$$

with inverse

$$(6.9) \quad J(u, v)^{-1} = \frac{1}{2} \begin{pmatrix} -\exp(u - v) & -\exp(u + v) \\ \exp(u - v) & -\exp(u + v) \end{pmatrix}.$$

Thus, if  $x^* = (u^*, v^*)$  satisfies (6.7), then

$$(6.10) \quad Y = J(u^*, v^*)^{-1} = \begin{pmatrix} -5 & -5 \\ 5 & -5 \end{pmatrix}$$

is obtained without knowing  $x^*$ . Using (6.10), the iteration process (1.3) for  $\phi$  given by (5.1) with  $f$  defined by (6.7) is

$$(6.11) \quad \begin{aligned} u_{n+1} &= u_n + 5\exp(-u_n)(\exp(v_n) + \exp(-v_n)) - 1, \\ v_{n+1} &= v_n - 5\exp(-u_n)(\exp(v_n) - \exp(-v_n)), \end{aligned}$$

which will converge quadratically if  $x_0 = (u_0, v_0)$  is close enough to  $x^* = (u^*, v^*)$  [19].

The choice  $x_0 = (4.3, 2.0)$  [4] leads to the results shown in Table 6.1. The calculations were done with an HP-33E pocket calculator, with rounding to four decimal places.

$n$	$u_n$	$v_n$	$\eta_n =  x_{n+1} - x_n $
0	4.3000	2.0000	0.4921
1	3.8105	1.5079	0.4755
2	3.3350	1.0324	0.4366
3	2.8984	0.5958	0.3481
4	2.5503	0.2477	0.1954
5	2.3549	0.0524	0.0498
6	2.3052	0.0026	0.0026
7	2.3026	6.9985 (-06)	-
8	2.3026	-4.6502 (-10)	-
9	2.3026	2.8499 (-10)	-
10	2.3026	2.8499 (-10)	-

Table 6.1. Numerical Results for the Iteration (6.11).

The elements of the iteration sequence  $\{x_n\}$  can be used to form cubes

$$(6.12) \quad x = (U, V) = x_n + 2\eta_n e \cdot [-1, 1] = (u_n \pm 2\eta_n, v_n \pm 2\eta_n),$$

which have the Krawczyk transformations

$$(6.13) \quad K(x) = x_{n+1} + \eta_n (I - YJ(U, V)) e \cdot [-1, 1],$$

using (5.4). Interval iteration starting with (6.12) as  $x_0$  and using (6.13) will stall

for  $n = 0, 1, 2, 3, 4$ . For  $n = 5$ , however, one gets

$$(6.14) \quad X_0 \supset K(X_0) = X_1 \supset K(X_1) = X_2 \supset K(X_2) = X_3,$$

with  $X_n = (U_n, V_n)$  given in Table 6.2.

$U_0 = 2.3549 \pm 0.0996$	$V_0 = 0.0524 \pm 0.0996$
$U_1 = 2.3052 \pm 0.0380$	$V_1 = 0.0026 \pm 0.0380$
$U_2 = 2.3026 \pm 0.0046$	$V_2 = 0.0000 \pm 0.0046$
$U_3 = 2.3026 \pm 0.00002$	$V_3 = 0.0000 \pm 0.00002$

Table 6.2. Results of Interval Iteration.

The results given here verify the existence of  $x^* \in X_n$ ,  $n = 0, 1, 2, 3$ , and the approximate solution  $x = (2.3026, 0.0000)$  is guaranteed to be accurate to four decimal places, since  $x = m(X_3)$ ,  $\frac{1}{2}w(X_3) = 0.00002$ . The calculations here were also done using an HP-33E, with the subroutines [23] augmented by simple programs for  $\exp(X)$  and  $\exp(-X)$ , and, of course, directed rounding of the results to the number of places indicated in the table.

7. The eigenvalue-eigenvector problem. Interval iteration can also be applied to the *eigenvalue-eigenvector problem* for a real matrix  $A$ , which is to find real numbers  $\lambda$  and corresponding nonzero vectors  $x$  such that

$$(7.1) \quad Ax - \lambda x = 0.$$

The condition  $x \neq 0$  is often enforced by a *normalization* of  $x$ ,

$$(7.2) \quad (a) \quad (x, x) - 1 = 0, \quad \text{or} \quad (b) \quad (a, x) - 1 = 0,$$

the latter for a fixed vector  $a$ . The system of equations formed by (7.1) and (7.2)(a) or (7.2)(b) is a nonlinear system of  $v + 1$  equations in the  $v + 1$  unknowns  $x_1, x_2, \dots, x_v, \lambda$ . In fact, the result is a special case of what are called *quadratic systems* of equations, in which the transformation  $f(x)$  has the form

$$(7.3) \quad f(x) = Bxx + Lx + c,$$

in which  $B = (b_{ijk})$  is a *bilinear operator*,  $L$  is a given matrix, and  $c$  is a fixed

vector [17], [20]. The derivative of the quadratic operator  $f$  defined by (7.3) is

$$(7.4) \quad f'(x) = 2\bar{B}x + L,$$

where  $\bar{B} = \frac{1}{2}(b_{ijk} + b_{ikj})$  is a symmetric bilinear operator [17], [20]. It follows that

$$(7.5) \quad F'(X) = 2\bar{B} \cdot X + L$$

gives an interval extension of (7.4), furthermore, since  $\bar{B}$  is a linear operator on  $x$  (into the space of matrices), one has

$$(7.6) \quad m(F'(X)) = 2\bar{B}m(X) + L = F'(m(X)),$$

which means that the Newton form (5.6) and the Moore-Jones form (5.9) of the Krawczyk iteration operator will coincide for quadratic systems of equations. Thus, an interval iteration method based on Newton's method will have a simple computational form in this case. In particular, the formulation of the eigenvalue-eigenvector problem (7.1) as a system of quadratic equations [2], [18] leads to a simple interval iteration method, which will be given below.

Returning to (7.1), if  $x^* \neq 0$  is an eigenvector of  $A$ , then the corresponding eigenvalue  $\lambda^*$  is given by the Rayleigh quotient

$$(7.7) \quad \lambda^* = R(x^*) = (Ax^*, x^*) / (x^*, x^*).$$

Consequently, if  $x^* \in X$  for some interval vector  $X$  such that  $0 \notin X$ , then the interval Rayleigh quotient

$$(7.8) \quad R(X) = (AX, X) / (X, X)$$

can be used to obtain lower and upper bounds for  $\lambda^*$ : Since  $\lambda^* \in R(X) = [c, d]$ , it follows that

$$(7.9) \quad c \leq \lambda^* \leq d.$$

$R(X)$  can be computed automatically, using interval arithmetic, with the extension

$$(7.10) \quad (x, x) = \sum_{i=1}^n x_i^2$$

of  $(x, x)$ , where the square of an interval is defined to be

$$(7.11) \quad [a, b]^2 = \begin{cases} [\min\{a^2, b^2\}, \max\{a^2, b^2\}] & \text{if } ab \geq 0, \\ [0, \max\{a^2, b^2\}] & \text{if } ab < 0. \end{cases}$$

Formula (7.11) gives a better extension of  $f(x) = x^2$  than  $F(X) = X \cdot X$  for intervals  $X$  which contain both positive and negative numbers; for example,  $[-1,1]^2 = [0,1]$ , while  $[-1,1] \cdot [-1,1] = [-1,1]$ .

The eigenvalue-eigenvector problem for  $A$  will be considered in the form of the quadratic system (7.1)-(7.2)(b). Eigenvectors orthogonal to  $a$  will not satisfy this system, but can be obtained from a system with a different choice of  $a$ . It will be shown that the Krawczyk transformation required to apply interval iteration to this problem can be expressed as the sum of the point obtained by Newton's method [2], [18], and an easily computed symmetric interval vector.

Following [18],  $a$  will be taken to be a unit vector in (7.2)(b), for example,  $a = (0, \dots, 0, 1)$ . This gives  $x_v = 1$ , and (7.1)-(7.2)(b) becomes the system of  $v$  equations

$$\begin{aligned}
 (a_{11} - \lambda)x_1 + a_{12}x_2 + \dots + a_{1,v-1}x_{v-1} + a_{1v} &= 0, \\
 a_{21}x_1 + (a_{22} - \lambda)x_2 + \dots + a_{2,v-1}x_{v-1} + a_{2v} &= 0, \\
 \dots & \\
 a_{v-1,1}x_1 + a_{v-1,2}x_2 + \dots + (a_{v-1,v-1} - \lambda)x_{v-1} + a_{v-1,v} &= 0, \\
 a_{v1}x_1 + a_{v2}x_2 + \dots + a_{v,v-1}x_{v-1} + a_{vv} - \lambda &= 0,
 \end{aligned}
 \tag{7.12}$$

for the  $v$  unknowns  $x_1, x_2, \dots, x_{v-1}, \lambda$ . The derivative  $f'$  of the operator  $f$  defined by the left side of (7.12) is

$$f'(\xi) = \begin{pmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1,v-1} & -x_1 \\ a_{21} & a_{22} - \lambda & \dots & a_{2,v-1} & -x_2 \\ \dots & \dots & \dots & \dots & \dots \\ a_{v-1,1} & a_{v-1,2} & \dots & a_{v-1,v-1} - \lambda & -x_{v-1} \\ a_{v1} & a_{v2} & \dots & a_{v,v-1} & -1 \end{pmatrix},
 \tag{7.13}$$

where  $\xi = (x_1, \dots, x_{v-1}, \lambda)$ . An interval extension  $F'(\Xi)$  of (7.13) is obtained by simply replacing  $f$  by the interval vector  $\Xi = (X_1, \dots, X_{v-1}, \Lambda)$ . Since most of the components

of  $F'(\Xi)$  are real numbers, the real matrix  $w(F'(\Xi))$  has the simple form

$$(7.14) \quad w(F'(\Xi)) = \begin{pmatrix} w(\Lambda) & 0 & \dots & 0 & w(X_1) \\ 0 & w(\Lambda) & \dots & 0 & w(X_2) \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & w(\Lambda) & w(X_{v-1}) \\ 0 & 0 & \dots & 0 & \dots \end{pmatrix}.$$

Thus, the vector  $w(F'(\Xi))w(\Xi)$  is given by

$$(7.15) \quad w(F'(\Xi))w(\Xi) = 2w(\Lambda)(w(X_1), \dots, w(X_{v-1}), 0) = 2w(\Lambda)w(X^{(v)}),$$

where  $X^{(v)} = (X_1, \dots, X_{v-1}, 0)$ . For  $Y = \{f'_i\}$ ,  $\eta = m(\Xi)$ , the transformation

(5.9) becomes

$$(7.16) \quad K(\Xi) = \eta - Yf(\eta) + \frac{w(\Lambda)}{2} |Y| w(X^{(v)}) \cdot [-1, 1],$$

the sum of the Newton point  $\zeta = \eta - Yf(\eta)$  and a simply computed symmetric interval vector. Formula (7.16) simplifies further for  $w(X_1) = w(X_2) = \dots = w(X_{v-1}) = 2\rho$ , one has

$$(7.17) \quad K(\Xi) = \eta - Yf(\eta) + \rho w(\Lambda) |Y| e^{(v)} \cdot [-1, 1],$$

where  $e^{(v)} = (1, \dots, 1, 0)$ .

An alternative method for obtaining lower and upper bounds for eigenvalues of  $A$  is available from (7.12). If  $x^* \in X = (X_1, \dots, X_{v-1}, 1)$  is an eigenvector of  $A$ , then  $\lambda^* \in \Lambda$  for the corresponding eigenvalue  $\lambda^*$ , where

$$(7.18) \quad \Lambda = a_{vv} + \sum_{j=1}^{v-1} a_{vj} \cdot X_j$$

is the interval version of the last equation of (7.12). The use of this expression and the interval Rayleigh quotient  $R(X)$  given by (7.8) to obtain bounds for eigenvalues of matrices will be illustrated in the example below.

Consider the simple example

$$(7.19) \quad A = \begin{pmatrix} 3 & 1 & -1 \\ 1 & 5 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

Here, system (7.12), written for  $\xi = (u, v, \lambda)$ , becomes

$$(7.20) \quad \begin{aligned} 3u + v - \lambda u - 1 &= 0, \\ u + 5v - \lambda v - 1 &= 0, \\ -u - v - \lambda + 3 &= 0. \end{aligned}$$

For the initial approximations  $u_0 = v_0 = 1$ , the third equation of (7.20) gives  $\lambda_0 = 1$ . The results of applying Newton's method to (7.20), starting from  $\xi_0 = (1, 1, 1)$ , are shown in Table 7.1. These are rounded to four places from a double-precision calculation performed on a UNIVAC 1160, using the program NEWTON [6].

n	$u_n$	$v_n$	$\lambda_n$
0	1.0000	1.0000	1.0000
1	0.8182	0.2727	1.9091
2	0.9755	0.0166	2.0079
3	1.0002	-0.0001	1.9999
4	1.0000	0.0000	2.0000

Table 7.1. Results of Newton's Method.

In order to construct an interval  $\Xi$  to which to apply the Krawczyk transformation (7.17), it is helpful to split the vector  $\xi$  into its *vector-like* part  $\xi^{(v)} = (x_1, x_2, \dots, x_{v-1}, 0)$ , and its *value-like* part  $\xi_v = (0, \dots, 0, \lambda) = \lambda e_v$ ,  $e_v = (0, \dots, 0, 1)$ . Then, for

$$(7.21) \quad \eta_0 = \|\xi_{n+1}^{(v)} - \xi_n^{(v)}\|_\infty,$$

it is reasonable to choose  $\rho = 2\eta_0$ ,  $w(\lambda) = 4|\lambda_{n+1} - \lambda_n|$ . This gives

$$(7.22) \quad \Xi = \xi_n + 2\eta_0 e^{(v)} \cdot [-1, 1] + \frac{1}{2} w(\lambda) e_v \cdot [-1, 1]$$

as the interval to be examined. Splitting the vector

$$(7.23) \quad t = |Y|e^{(v)} = |[m(F'(\Xi))]^{-1}|e^{(v)} = t^{(v)} + t_v = t^{(v)} + t e_v,$$

it follows from (7.17) that the condition  $K(\Xi) \subset \Xi$  will hold if the inequalities

$$(7.24) \quad \eta_0 \leq 1/2\tau, \quad |\lambda_{n+1} - \lambda_n| \leq 1/8\|t^{(v)}\|_\infty$$



are satisfied. Observation of the sequence given in Table 7.1 shows that (7.24) holds for  $n = 1$ , thus, for

$$(7.25) \quad \Xi = \begin{pmatrix} 0.8182 \\ 0.2727 \\ 1.9091 \end{pmatrix} \pm \begin{pmatrix} 0.5122 \\ 0.5122 \\ 0.3952 \end{pmatrix} = \begin{pmatrix} [0.3060, 1.3304] \\ [-.2395, 0.7849] \\ [1.5139, 2.3043] \end{pmatrix},$$

one has

$$(7.26) \quad |Y|e^{(3)} = \begin{pmatrix} 1.1289 \\ 0.9075 \\ 0.6761 \end{pmatrix}, \quad K(\Xi) = \begin{pmatrix} [0.7469, 1.2041] \\ [-.1671, 0.2003] \\ [1.8710, 2.1448] \end{pmatrix} \subset \Xi.$$

The non-negative numbers entering into the calculation have, of course, been rounded upward to four decimal places, so that (7.26) proves that the matrix  $A$  given by (7.19) has an eigenvector  $x^* = (x_1^*, x_2^*, 1)$  and a corresponding eigenvalue  $\lambda^*$  which satisfy

$$(7.27) \quad 0.7469 \leq x_1^* \leq 1.2041, \quad -.1671 \leq x_2^* \leq 0.2003, \quad 1.8710 \leq \lambda^* \leq 2.1448,$$

since  $\xi^* \in K(\Xi)$ , and the interval iteration using the transformation (7.17) will converge. The interval Rayleigh quotient applied to  $X = ([0.7469, 1.2041], [-.1671, 0.2003], 1)$  obtained from  $K(\Xi)$  in (7.26) gives

$$(7.28) \quad R(X) = [0.8752, 3.8826],$$

while formula (7.18) gives

$$(7.29) \quad \Lambda = [1.5956, 2.4202].$$

The bounds that (7.28) and (7.29) provide for  $\lambda^*$  are rigorous, but inferior to (7.27) in this case.

The transformation (7.17) can also be used to check the final result  $\xi_4$  of the numerical computation given in Table 7.1. Take, for example,

$$(7.30) \quad \Xi = \xi_4 + 0.0001e \cdot [-1, 1],$$

so that  $\rho = 0.0001$ ,  $w(\Lambda) = 0.0002$ . Since  $|Y|e^{(3)} = e$  for these values, one has

$$(7.31) \quad K(\Xi) = \xi_4 + 0.0000002e \cdot [-1, 1] \subset \Xi,$$

which proves that the components of  $\xi_4$  are accurate to six decimal places. Of course, the numerical iteration process stumbled onto the exact solution  $\xi^* = \xi_4$  in this case, but this fact is not required for the rigorous error analysis (7.31).

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) In actual practice, iteration methods applied to the solution of finite systems of equations yield inconclusive results as to the existence or nonexistence of solutions and the accuracy of any approximate solutions obtained. On the other hand, construction of interval extensions of ordinary iteration operators permits one to carry out interval iteration computationally, with results which can give rigorous guarantees of existence or nonexistence of solutions, and error bounds for approximate solutions. Examples are given of the solution of a nonlinear system of equations and the calculation of eigenvalues and eigenvectors of a matrix by interval iteration. Several ways to obtain lower and upper bounds for eigenvalues are given.		

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